(1R,2S,5R)-(-)-Menthol
2216-51-5 | DTXSID1022180

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 214 °C

Global applicability domain: Inside

Local applicability domain index: 9.72e-01

Confidence level: 8.89e-01

Nearest Neighbors from the Training Set

Image not found
Menthol
Measured: 212
Predicted: 214

Image not found
Cyclohexanol, 1-methyl-4-(1-methylethyl)-
Measured: 209
Predicted: 214

Image not found
Citronellol
Measured: 224
Predicted: 223

Image not found
Citronellol
Measured: 224
Predicted: 223